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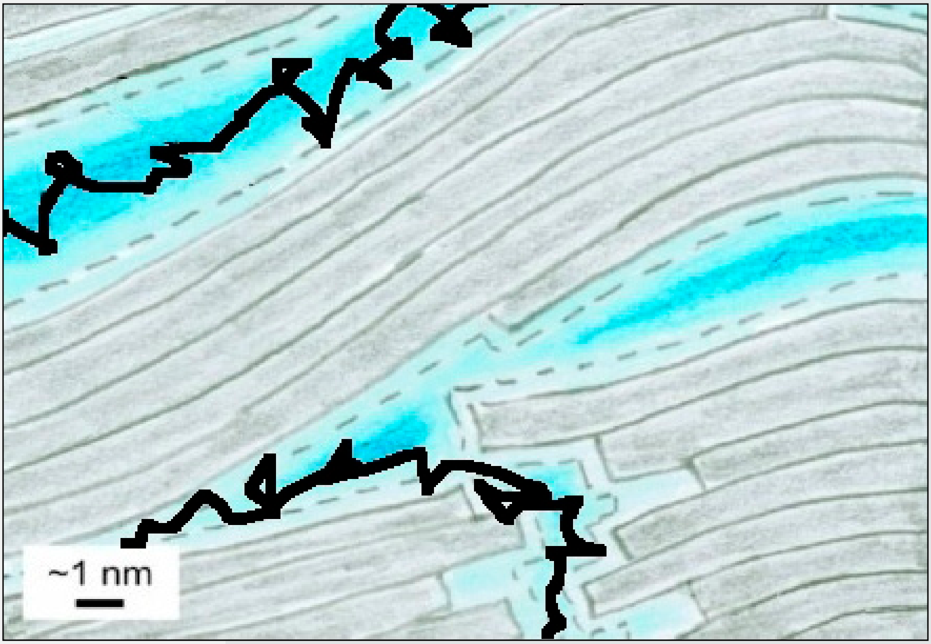

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Société Suisse pour la Diffusion des Neutrons
Swiss Neutron Scattering Society

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ON THE COVER:

Macroscopic pore structure of clays. Black lines show the diffusion paths schematically, see related article by F. Juranyi et al within this issue. Courtesy: ‘Sondierbohrung Benken, Untersuchungsbericht, Nagra Technical Report, NTB 00-01. Wettingen, Switzerland.’

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The President's Page

DEAR MEMBERS

A big step from neutron dream to neutron reality has been made by the decision to site the ESS in Lund, Sweden. In this issue, I would like to quote myself on this subject as the chairman of ENSA as this will be my last editorial as president of the Swiss Neutron Scattering Society:

"The decision on where the ESS should be built has been eagerly awaited by thousands of European scientists whose research depends so crucially upon neutrons. Three extremely good candidates, Sweden, Spain and Hungary, proposed excellent sites to host the ESS. Each of their campaigns strongly emphasised both the strategic importance of the ESS for European science, and the urgency to build the ESS in light of the new American and Japanese spallation neutron sources.

Unfortunately, it has always been agreed upon that only one of the three candidate sites could ultimately host the ESS. In this respect European Research ministers recommended that the ESS site should be in Lund in Sweden. Spain has already graciously pledged to exploit the expertise and momentum it has gained in the last three years by signing an agreement to help ESS-Scandinavia deliver the ESS that Europe needs.

We hope that Hungary will similarly follow this initiative and actively bring its expertise to the ESS table. In this way there is potential for all three serious site contenders to benefit from their dedication and commitment over the last few years. There is, however, no doubt that, in general, European neutron scatterers and European science will benefit!

On behalf of Europe's neutron users, represented by the European Neutron Scattering Association, ENSA, I would like to extend my thanks and admiration to the Swedish, Spanish and Hungarian teams and also to all the other neutron scientists and technologists from across Europe who are continuing to work so hard to turn the ESS from neutron dream to neutron reality."

This decision makes it easy for me to step down as president of the SGN/SSDN and as chairman of ENSA and to look back on the huge work done by numerous people in the community in order to achieve this decision. The Swiss community played a very important role in this and it will do so, I 'm sure, also in the realisation phase of the ESS. The active participation of you in the project at any level will allow that the Swiss participation in the ESS will be assured and justified.

Peter Allenspach

Linking the Diffusion of Water in Clays at Different Time and Length Scales: Insights from Quasielastic Neutron Scattering and Tracer Through-Diffusion

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CLAYS

Clay minerals are aluminium phyllosilicates, mostly products of chemical weathering or hydrothermal alteration of igneous and metamorphic rocks. Their layered, fine-grained structure can be directly related to their physical and chemical properties. These properties such as large water retention, low hydraulic conductivity, heat resistance and ionic exchange capacities, make clays ideal for many different applications, e.g. concrete, brick, paper and ceramics production, in catalysis, or as sealing material for the underground disposal of radioactive waste.

The long-term disposal of radioactive waste in an underground geological repository is based on a multibarrier concept. In the barrier of highly compacted clay, water is intercalated and confined between the clay layers. The narrow pores mean that under natural hydraulic gradients, molecular diffusion through the pore water is the dominant transport mechanism for released radionuclides. A large number of studies agreed that the properties of water at the water-clay interface differ from those of bulk water. In order to predict the transfer of solutes through a clay barrier, a good and deep understanding of the water structure and dynamics in compacted clay systems is fundamental.

The mineralogy and structure of clays as well as the mechanisms governing the water-clay system have been described extensively in the literature over the last decades. Clay minerals are built up of a number of crystalline sheets (Fig. 1) having either tetrahedral (T) or octahedral (O) symmetry. Two or three such sheets form a TO or TOT layer. Isomorphic substitution (replacement of ions in the crystals without change of the structure) may occur in any of these sheets. As a result a negative layer charge is developed which is compensated by cations in the interlayer space and on or near the external surfaces. Several sequences of TO, TOT layers are combined and form larger units called stacks. Several clay stacks group together to produce particles and aggregates (Fig. 2). The density and location of the isomorphic substitutions and the type of the compensating cation determine the layer stacking of a clay particle and the behaviour of the particle when hydrated.

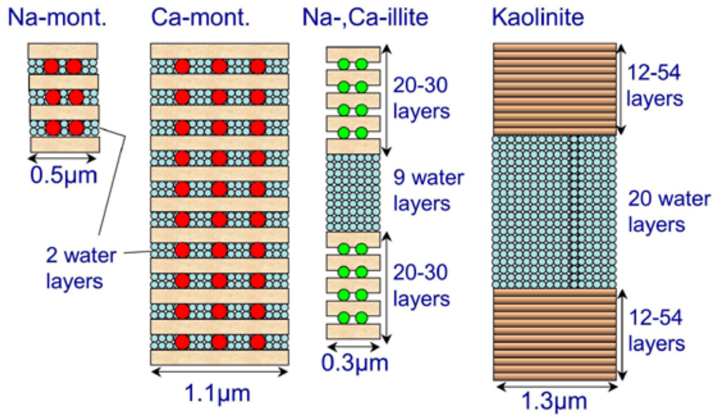

Fig. 1. Microscopic structure of the investigated clays. Depending on the type of the clay, water can be located in the interlayer (Na- and Ca-montmorillonite) or at tetrahedral (Na- and Ca-illite and kaolinite) or octahedral (kaolinite) crystalline surfaces. Blue balls represent water, green balls Potassium, and red balls Na or Ca ions. The clay sheets have TO structure in the case of kaolinite and TOT in the others.

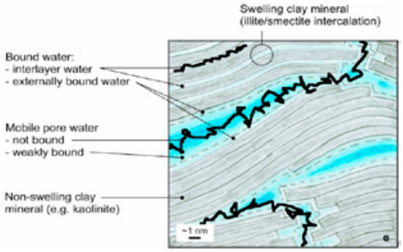

Fig. 2. Macroscopic structure of clays. Black lines show the diffusion paths schematically. Courtesy: 'Sondierbohrung Benken, Untersuchungsbericht, Nagra Technical Report, NTB 00-01. Wettingen, Switzerland.'

Water can be located in larger pores between the stacks and/or in the interlayer. When water enters in the interlayer, the interlayer space increases and the clay swells. X-ray diffraction patterns showed that swelling occurs stepwise at low hydration [1], therefore one can speak about clays with, on average, 1, 2 or 3 layers of water in the interlayer.

DIFFUSION AT DIFFERENT TIME-SCALES

The water diffusivity in clays is affected by the geometrical microstructure of the pore network, that is, porosity, tortuosity, constrictivity, and by the interaction between water and clay. There are some empirical and theoretical models which relate the effective diffusion coefficient with the porosity and water content in the porous medium [2, 3].

This article demonstrates the possibility of experimentally distinguishing geometric from chemical effects. The focus is on the importance of chemical effects on water diffusion in clays. Macroscopic tracer through-diffusion experiments measure diffusion over a length of centimeters (or more). The obtained value is the effective diffusion coefficient D_e, which can be related to the diffusion coefficient of bulk water D_w through the porosity ε, a geometry factor G, that mostly accounts for the tortuosity, and the electrostatic constraint q:

$$\mathbf{D_e = e/G\ q\ D_w} \quad (1)$$

On the microscopic scale the tortuosity effects are not relevant. Therefore, taking advantage of the much shorter observation time offered by quasielastic neutron scattering (QENS) it is possible to measure an averaged local diffusion coefficient D_l:

$$\mathbf{D_l = q\ D_w} \qquad (2)$$

According to our knowledge there are only two articles that compare diffusion coefficients obtained by macroscopic tracer diffusion and neutron scattering. Beyer et al. [4] obtained similar values for the two techniques, however the diffusion was bulk-like and not confined as in the present case. Rollet et al. investigated $N(CH_3)_4+$ diffusion in Naffion membrane with different experimental techniques [5]. They found, that the diffusion process inside Nafion cavities is similar to that in nonconfined solution. Furthermore, on long time scales the limiting factor of the diffusion is the transfer through the pores which connect cavities. However in case of clays the process of water diffusion must be different because of the pore geometry.

MATERIALS

Three different types of pure clays, montmorillonite (in Na- and Ca-form), illite (in a Na- and Ca-form) and kaolinite have been investigated at high compaction states (bulk dry density of 1.9±0.05g/cm^3). Their structural differences (Fig. 1) result in significantly different behaviour when they are in contact with water. In the case of montmorillonite at the given compaction, water is located mainly in the interlayer space. In illite, water is found only between particles, because the interlayer surfaces are tightly linked by potassium cations. The layers of kaolinite are uncharged and therefore have no interlayers; thus water is likewise located only between particles (Fig. 2).

The studies of the diffusion coefficient were accomplished by careful and detailed characterization of the clay samples using various methodologies to better interpret the data. Parameters such as particle size, layer spacing, chemical composition, external and total surfaces and porosity were determined [6].

DIFFUSION AT THE MICROSCOPIC SCALE STUDIED BY QUASIELASTIC NEUTRON SCATTERING

Quasielastic neutron scattering experiments were performed on different instruments using different setups to vary the energy resolution, which is a key parameter for the data analysis. The parameters obtained for the diffusion were consistent, a feature that supports their validity. The most critical point in the data treatment is the choice of an appropriate model, as this step may introduce systematic errors. We applied some possible models from the literature to estimate this error. The measurements have been performed from 95°C down to –23°C in the case of illites and montmorillonite, and down to room temperature in case of kaolinite.

The systematic differences in the clay structures were reflected in the water diffusion[7]. Charged clays had lower diffusion coefficients D than kaolinite, which had similar (or even higher) diffusion coefficients than that of bulk water. Within the charged clays the swelling clays like Na- and Ca-montmorillonite were found to clearly reduce water diffusion, a property which is attributed to their particular confining interlayer structure. The water diffusivity in these two types of montmorillonite was similar. Because most water molecules are located in the interlayer, diffusive motion seems to be more strongly affected by the geometrical confinement than by the difference in the saturating cation (Na^+ or Ca^{2+}). However, when the cations are located on the external surfaces, and their concentration is lower in the solution, as it is in the case of illite, there is a significant difference in water diffusion between the Ca- and Na-forms. Calcium ions reduce water mobility in illite more strongly than Na^+, as they are also known to do in aqueous solutions [8].

Similarly to aqueous solutions, the activation energy of water diffusion in Ca-illite was larger than in the Na-form owing to its stronger propensity to order the water molecules (cosmotrope character) [9]. This was not observed in montmorillonite because of its strong interlayer confinement. The above mentioned qualitative differences have been observed over the whole investigated temperature range.

DIFFUSION AT THE MACROSCOPIC SCALE STUDIED BY TRACER THROUGH-DIFFUSION

The effective diffusion coefficients have been obtained in the temperature range between 0 and 60°C. Over the entire temperature range they followed the order Na-montmorillonite < Ca-montmorillonite < Ca-illite < Na-illite ≤ kaolinite [6]. The differences were interpreted in accordance with the independently estimated structural properties of the samples (see also Figs. 1 and 2). These showed that Na-montmorillonite had the smallest particle and pore sizes and thus was expected to have the largest tortuosity and therefore the lowest effective diffusion coefficient. Na-montmorillonite was followed by Ca-montmorillonite, the illites, and kaolinite. The differences between the two forms of illite, which have similar stacking structures, were interpreted to originate from differences in the solvation of Na and Ca ions. Activation energies larger than those of bulk water were found for the montmorillonites, whereas values similar or slightly lower than those of bulk water were found for the illite and the kaolinite clays.

COMPARISON OF THE RESULTS

Since QENS has an observation time on the order of picoseconds, the translational diffusion coefficients obtained at this microscopic scale are determined by local effects. Tracer through-diffusion experiments (across the whole sample) are additionally influenced by the mesoscopic – macroscopic pore structure of the clays.

The large difference in the diffusion paths of the two selected techniques therefore renders a direct comparison of water diffusivities impossible. Nevertheless, two means to compare the results could be established [10]:

- An indirect comparison is enabled by connecting the diffusion coefficients at the two different scales through the geometrical factor G and the electrostatic constraint q;
- and a direct comparison is possible via the activation energy E_a.

DIFFUSION COEFFICIENTS

Na- and Ca- illite have a very similar structure owing to their similarities in porosity and particle size and in the way they produce stacks of 20-30 particles [11]. Differences in the diffusion between the illites should therefore be dominated by the electrostatic constraint. In contrast, the geometrical factors for the montmorillonites should be different because of the different particle size and stacking. The obtained q and G factors (Tab. 1) nicely reflect the expected behaviours, lending confidence to this method of comparison for this type of porous materials.

ACTIVATION ENERGY

It is known that the temperature dependence of water diffusion can only be described approximately by the Arrhenius law. However it yielded to a good description of our data for temperatures above 0 °C. For the clays with larger pores (illites and kaolinite) a very good agreement was found between Ea values obtained by the two methods. In both montmorillonites, however, where the majority of the water molecules are located in a kind of double-layer between the clay sheets,

	$q = D_{l\,(QENS)}/D_{bulk\ water\ (QENS)}$	$G = \varepsilon D_{l\,(QENS)}/D_{e\ (tracer\ diff.)}$
Na-illite	0.9 ± 0.1	3.9 ± 0.4
Ca-illite	0.6 ± 0.1	4.2 ± 0.4
Na-montmorillonite	0.5 ± 0.2	21.0 ± 2.0
Ca-montmorillonite	0.5 ± 0.1	8. ± 0.8
Kaolinite	1.2 ± 0.2	4.6 ± 0.5

Table 1. Electrostatic constraint, q and geometrical factor, G obtained from the quasielastic neutron scattering and tracer through-diffusion experiments at 20 °C. Since the experiments were not done at the same temperature, the values have been extrapolated according to the observed Arrhenius behaviour.

the activation energy obtained from the tracer through-diffusion measurements was much larger than that found by the QENS experiments. For these clays there is not even a qualitative agreement between the two methods: in comparison to the other clays the montmorillonites have the lowest activation energy according to the QENS but the highest according to the tracer diffusion experiment. It is clear that the QENS data describe only local movements. The different activation energies for montmorillonite at the two scales may hint to a specific scale dependence of the diffusion in this clay. This scale dependence could, for instance, originate from a coupling between the motion of water and the cations that only becomes relevant at the macroscopic scale.

We conclude that the geometrical factor and the electrostatic constraint can be determined by comparing the diffusion coefficients measured by the two different techniques; tracer through-diffusion and QENS.

Furthermore, activation energies obtained at the two scales are similar for clays having no interlayer water (non-swelling clays such as the illites and kaolinite). For montmorillonite the Ea values are different. Further investigations are required to clarify the reasons for these differences.

The authors are thankful to Georg Kosakowski, Bart Baeyens, Martin Glaus and Andreas Jakob for fruitful discussions and to Werner Müller for the help in the laboratory. The neutron scattering experiments were performed at PSI and FRM II. We acknowledge the beam time and the help of Tobias Unruh, who was the local contact at FRM II.

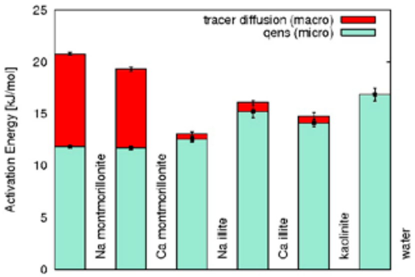

Fig. 3. Activation energy for water diffusion in different clays measured by tracer through-diffusion and quasielastic neutron scattering

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Self-Diffusion Studies in Solids Using Neutron Reflectometry

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Neutron reflectometry can be used to study self-diffusion processes in solids on the sub-nanometer scale. This allows the detection of ultra-low diffusivities down to 10^{-26} m^2/s. Using neutron reflectometry, the extensive characterization of materials which are in a non-equilibrium state, like amorphous or nano-crystalline solids becomes possible, as well as diffusion studies in ultra-thin films and at low temperatures. We illustrate the basic aspects and potential of this technique for different classes of materials: amorphous silicon nitride, nano-crystalline iron, and single crystalline germanium.

INTRODUCTION

The investigation of self-diffusion in solids is one of the most fundamental tasks in materials science and materials physics. Diffusion is an important point-defect mediated matter transport process and self-diffusivities, *D*, are a measure for the mobility of the constituting atoms in all kind of materials. Various processes in solids, which are important for the tailoring of materials properties and thermal stability are controlled by self-diffusion. Typical examples are mechanical deformation [1], grain growth [2], oxide layer growth [3], ion conductivity [4], crystallization and precipitation [5].

Common methods which are generally used for the study self-diffusion are methods based on radioactive or stable tracers combined with adequate depth profiling (SIMS, NRA), nuclear magnetic resonance (NMR), quasielastic neutron scattering (QENS) and Mößbauer spectroscopy [6]. Using these methods self-diffusivities over 13 orders of magnitude in the range from 10^{-23} to

10^{-10} m^2/s can be derived, which may serve as input parameters in various process simulations and models.

During the last years a new interesting method was developed for the determination of ultra-low diffusivities down to 10^{-26} m^2/s and ultra-short diffusion lengths, ($d = (2\ D\ t)^{1/2}$), of 1 nm and below. This method is based on the application of neutron reflectometry on isotope multilayers [7-10].

The main advantage of this method is that small detectable diffusion lengths allow the extensive characterization of metastable solids, like amorphous and nano-crystalline materials. For a successful diffusion experiment in nanomaterials the diffusion length has to be considerably below the typical dimensions of the nanosized building blocks or structure units (e. g. grains, domains etc.). Otherwise, diffusion controlled processes like e. g. grain growth lead to a significant modification of the actual nanostructure during the diffusion experiment on the scale of the diffusion length. A similar argument is true for glasses or amorphous semiconductors. Here, during diffusion annealing atomic re-arrangements in the order of the diffusion length may take place, which induce nucleation and growth, modifying the structural state wherein diffusivities should be determined. Furthermore the method also allows an expansion of the dynamic range in which diffusivities can be determined down to considerable low temperatures. If the diffusion length is reaching atomic distances, new tasks in fundamental diffusion research are possible.

In the present paper we give an overview on recent neutron reflectometry experiments of our group.

ISOTOPE MULTILAYERS

For diffusion experiments, the samples have to be prepared in form of isotope multilayers. These are thin films, which are deposited on a suitable substrate (e. g. a silicon wafer) by sputtering or molecular beam epitaxy. The isotope multilayers are composed of an alternating sequence of nanometre sized ^{n}AB and ^{m}AB layers, where A and B are the components of a certain chemical compound and n and m are the mass numbers of different stable isotopes of A. This arrangement is chemically completely homogenous, but isotope modulated (see Fig. 1). If the two isotopes ^{n}A and ^{m}A have sufficiently different coherent neutron scattering lengths, the isotope interfaces become sensitive to neutron scattering.

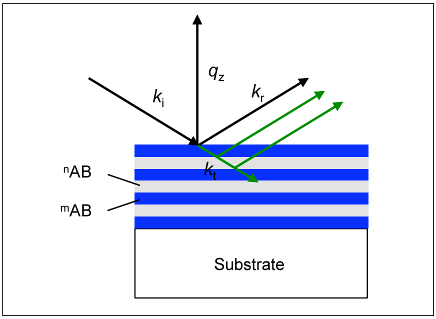

Fig. 1. Schematic sketch of an isotope multilayer. Also shown are the wave vectors, k, for specular neutron scattering (i: incoming, r: reflected, t: transmitted) and the scattering vector, q_z.

NEUTRON REFLECTOMETRY

During neutron reflectometry measurements a beam of cold neutrons is directed on the isotope hetrostructure surface at small incident angles below 2° (see Fig. 1). The neutron beam is now reflected at the film surface and at the film/substrate interface but also at interfaces existing between the various isotope layers. This gives rise to interference effects, which can be detected. In the reflectivity pattern, Bragg peaks are formed due to reflection at an artificial one-dimensional "isotope lattice" (see Fig. 2 (a)). Annealing of such an arrangement at elevated temperatures gives rise to isotope interdiffusion without modifying chemical composition and pure self-diffusion can be measured. During annealing, the Bragg peaks decays according to [11]

$$\mathbf{I(t) = I(0)exp\left(- \frac{8\pi^2 n^2 D}{l^2} t\right)} \quad (1)$$

where $I(t)$ is the intensity of the nth order Bragg peak at time t, and l is the bi-layer thickness. From this intensity decrease diffusivities, D, can be calculated.

Neutron reflectometry measurements were carried out at the Swiss spallation neutron source (SINQ) at the time-of-flight reflectometer AMOR using incoming neutron wavelengths between 0.2 and 0.9 nm [12]. Additional measurements were done at the Geesthacht Neutron Facility (GeNF) using the monochromatic (0.64 nm) reflectometer PNR.

SELF-DIFFUSION IN AMORPHOUS COVALENT SOLIDS

Covalently bound amorphous solids (e. g. silicon (carbo-)nitrides) are interesting light weight materials for functional and structural high temperature applications [13] with isotropic properties. The covalent bonds result in an excellent high temperature stability but also extremely low self-diffusivities [14]. Characterization of solid state kinetics necessitates the detection of extremely short diffusion lengths in order to prevent an overlapping of crystallization and diffusion processes during annealing.

We carried out self-diffusion studies on the model system amorphous silicon nitride ($SiN_{1.3}$), using [$Si^{14}N_x/Si^{15}N_x$] isotope multilayers.

In Fig. 2 (a) the neutron reflectivity of an isotope multilayer is shown in comparison to a not isotope enriched amorphous SiN_x layer. As obvious, the isotope multilayer exhibits three Bragg peaks, which can be used for diffusion studies. In Fig. 2 (b) the decrease of the first order Bragg peak during isothermal annealing at 1150 °C is illustrated. The analysis of these data with Eq. (1) gives minimum diffusion lengths of 0.6 nm [11].

In order to understand the differences of self-diffusion in thermodynamically stable and unstable states (here: amorphous and crystalline) appropriate experiments were launched at AMOR [15,16]. Diffusivities in the relaxed amorphous state as a function of temperature are given in Fig. 3. in comparison to diffusivities measured for polycrystalline Si_3N_4 (grain size 80 nm). The experiments in the amorphous state were only possible by neutron reflectivity since very low diffusion length (0.6 to 6 nm) were necessary for successful results. The polycrystalline sample was prepared by in-situ crystallization of the amorphous one.

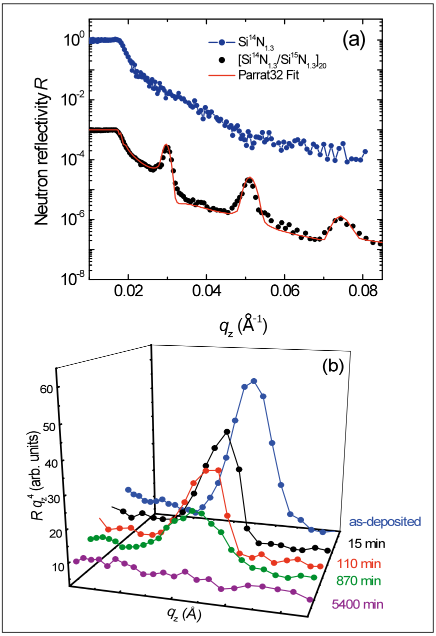

Fig. 2. (a) Neutron reflectivity pattern of a $[Si^{14}N_{1.3}(19\ nm)/Si^{15}N_{1.3}(6\ nm)]_{20}$ isotope multilayer compared to the pattern of a not enriched $Si^{14}N_{1.3}$ film. The reflectivity pattern of the multilayer is divided by a factor of 1000 for clarity [9]. (b) Decrease of the first order Bragg peak of a $[Si^{14}N_x(21nm)/Si^{15}N_x(7nm)]_{20}$ isotope multi-layer as function of annealing time during annealing at 1150 °C (after [15]).

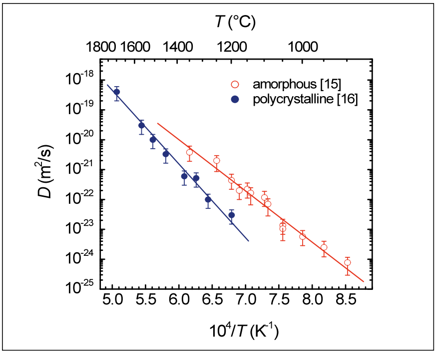

Fig. 3. Nitrogen diffusivities in polycrystalline Si_3N_4 (SIMS) [16] and amorphous $SiN_{1.33}$ (NR) [15] as a function of reciprocal temperature.

The diffusivities in the amorphous state are one up to two orders of magnitude higher than in the crystalline state in the temperature range investigated. Both types of data sets can be described by the Arrhenius equation

$$\mathbf{D = D_0 \exp\left(-\frac{H_i}{k_b T}\right)} \qquad (2)$$

with an activation enthalpy of $\Delta Ha = (3.6 \pm 0.4)$ eV for the amorphous state and of $\Delta Hc = (4.9 \pm 0.4)$ eV for the crystalline state, respectively. Diffusion in crystalline silicon nitride can be described by a mechanism based on thermal point defects (presumably interstitials) [16], where the activation enthalpy is the sum of a defect formation and defect migration part. However, for amorphous silicon nitride a direct mechanism based on structural point defects is suggested. Such structural point defects are left from strong structural relaxation processes and inherent to the amorphous structure. Consequently, a considerably lower activation enthalpy of diffusion is derived for the amorphous state [15], which is the result that the enthalpy of defect migration only is important here. The experiments should lead to a better understanding of polymorphous crystallization processes.

SELF-DIFFUSION IN NANO-CRYSTALLINE METALS

Nanocrystalline metals with small grain sizes of 5 – 100 nm show improved mechanical properties, like high hardness and fracture toughness. At low temperatures fundamental diffusion controlled processes like grain boundary creep, grain boundary sliding [1], grain growth [2] and also stress relaxation [17] are very important. Diffusion experiments with classical methods are hampered by the fact that simultaneous to the diffusion experiments significant grain growth takes place and the actual nanostructure is modified during annealing [18]. In order to quantify grain boundary self-diffusion in metals at low temperatures and in a stable nanostructure, we carried out self-diffusion measurements on nanocrystalline $[^{57}Fe/^{nat}Fe]_{10}$ isotope multilayers at AMOR (Fig 4 (a)). Transmission electron microscopy showed that the films are composed of columnar grains (about 30 nm x 160 nm) oriented perpendicular to the film surface. Diffusivities as a function of annealing time are given in Fig. 4 (b) for measurements at 400 °C.

Obviously, diffusivity depends drastically on time. It decreases by more than one order of magnitude with increasing annealing time. The diffusion lengths connected with these diffusivities range from of 1.1 – 1.6 nm, meaning that the present time-dependence of diffusivities cannot be detected by classical methods of diffusivity determination. The time dependence of the diffusivities can be explained to be the result of a point defect annihilation processes. At the beginning of the annealing process a large number of point defects are present in excess to the thermal equilibrium value, which were formed during sputter deposition and can be visualized as frozen-in non-equilibrium defects. Consequently, diffusion is governed by these excess point defects. During further annealing the number of point defects is reduced due to annihilation at sinks, a process which leads to a decrease of diffusivities. Since nano-crystalline metals are generally produced by non-equilibrium methods like inert gas condensation, ball milling, electro deposition or sputtering time-dependent diffusivities might be an inherent property of this materials class.

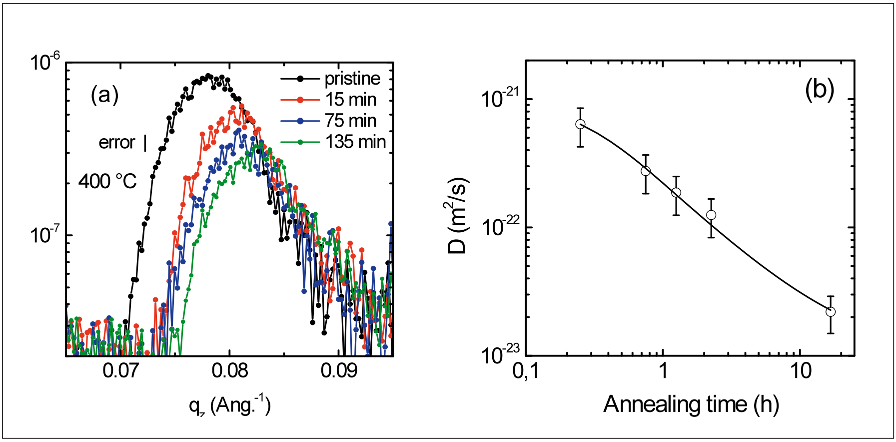

Fig. 4. (a) Decrease of the second order Bragg peak as a function of annealing time at 400 °C for magnetron sputtered $[^{57}Fe/^{nat}Fe]_{10}$ isotope multilayers. (b) Self-diffusivities in nano-crystalline Fe as a function of annealing time at 400 °C.

SELF-DIFFUSION IN SINGLE CRYSTALLINE GE

Single crystalline germanium is an important high mobility semiconductor with a high potential for future commercial fabrication of field effect transistors [19]. For device engineering it is necessary to obtain fundamental information on the properties of native point defects in Ge since nearly all technological important dopant atoms utilize these as diffusion vehicle.

The reflectivity of single crystalline [^{70}Ge/^{nat}Ge] multilayers was investigated at low temperatures between 430 and 600 °C [10] at PNR. The diffusivities, calculated according to Eq. (1) are presented in Fig. 5 in comparison to literature data. As obvious, at temperatures between 525 and 600 °C the diffusivities are in excellent agreement with literature data as measured by the radiotracer technique [20] or SIMS [21]. These results impressively demonstrate that our method gives diffusivities identical to those obtained by established methods.

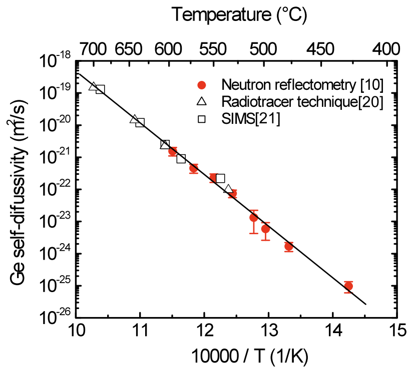

Fig. 5. Arrhenius plot of Ge self-diffusivities in comparison to literature data. The straight line is a fit of the NR data to Eq. (2) with $\Delta H = (3.13 \pm 0.12)$ eV and a pre-exponential factor of $D_0 = 2.35 \times 10^{-3}$ m^2/s (data of Ref. [10]).

However, significantly smaller diffusion lengths are measured (0.6 – 4.1 nm instead of 15 – 400 nm [20, 21]), meaning that diffusion lengths in the order of 1 nm characterize long range diffusion processes in this material in a correct way. At temperatures below 525 °C, additional diffusivities were measured by neutron reflectometry, expanding the range of experimental data by three orders of magnitude compared to sputtering techniques, forming an improved data base for process simulations. Note the ultra-low diffusivitiy of $D = (9.7 \pm 3.7) \times 10^{-26}$ m^2/s [10].

ACKNOWLEDGEMENTS

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9th International Conference on Quasielastic Neutron Scattering at PSI

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[2]Physical Chemistry, Saarland University, Saarbrücken, Germany

In February 2009 (10. – 13.02.2009) the 9th International Conference on QuasiElastic Neutron Scattering (http://qens2009.web.psi.ch/) took place at Paul Scherrer Institut (PSI) Villigen, Switzerland. The conference brought together participants from 14 countries : France (25%), Germany (18%), Switzerland (18%), USA (9%), Italy (8%), UK (7%) and other (15%) countries (Australia, India, Japan, Korea, Latvia, Poland, Russia, and Spain). The main topics of the conference have been confined matter, inclusion compounds and nanoporous materials, theory and numerical simulations, biological systems, polymers, glassy systems, molecular liquids, magnetic systems, and instrumentation. It became clear that biological topics, systems with and in confinement as well as complex fluids are the future trends in QENS.

4 plenary talks, 6 invited talks, 33 short presentations and 44 poster contributions provided an excellent overview about the progress and current topics in this field of research with neutrons. Prof. Alba–Simionesco (LLB, Saclay/France), showed in her plenary talk how a tree-point susceptibility can be used to extract the number of dynamically correlated particles during the structural relaxation. Prof. Chen (MIT, Cambridge/USA) discussed results on the pressure dependence of the dynamic crossover in confined supercooled water and its relation to the existence of a liquid-liquid critical point. The further theoretical developments in QENS and especially in the context of bio-matter have been emblazed by Prof. G. Kneller (Centre de Biophysique Moléculaire (CNRS, Orléans/France); he discussed the physical origin of fractional Brownian dynamics especially in the context of protein-solvent coupling. Finally Prof. G. Zaccai (ILL, Grenoble/France) reported in his plenary talk about the biological adaption to extreme temperatures and salt conditions in thermo- and hyperthermophile organisms.

From the number of presentations and posters related to biological and confined systems, it is clear that biophysically motivated topics as well as the research on systems in or with inherent confinements are attracting more and more scientific interest. By implication the increasing complexity of the systems under investigation claims for more sophisticated instruments (new instruments that are build or will be build in the very next future and the upgrade), also for more elaborated sample environments (like pressure, magnetic or electric fields and so on) and the combination of experimental data and results from computer simulations.

The social highlight was the conference dinner in Bad Zurzach. At this occasion three poster awards (in each case a book sponsored by Prof. Hempelmann / Saarland University, Germany) have been handed over to Veerendra Sharma (Bhabha Atomic Research Centre BARC /India) Tilo Seydel (ILL/France) and to Luis Carlo Pardo (Universitat Politecnica de Catalunya Barcelona /Spain) for their excellent poster contributions.

The conference proceedings will be published in "Zeitschrift für Physikalische Chemie" (Oldenbourg). Finally the 10th Conference on QuasiElastic Neutron Scattering has been decided to take place in 2012 in Nikko/Japan. We thank the school secretaries Mrs Renate Bercher and Mrs Pamela Knupp for the perfect organization and support before, during, and after the school. Financial support by PSI, EMPA, ILL, FRM-II, SwissNeutronics and Swiss National Science Foundation is gratefully acknowledged.

Jan Peter Embs (Conference Chairman) and
Fanni Juranyi (Scientific Secretary)

ENSA

The European Neutron Scattering Association

PRESS RELEASE (April 2, 2009)

2009 Walter Hälg Prize of the European Neutron Scattering Association (ENSA)

Every two years the European Neutron Scattering Association, ENSA, awards the prestigious Walter Hälg Prize to a European scientist for an outstanding programme of research in neutron scattering with a long term impact on scientific and/or technical neutron scattering applications. The Prize of 10’000 Swiss Francs is donated by Professor Walter Hälg, the founder of neutron scattering science in Switzerland. In 2009 the Walter Hälg Prize is to be presented at a special session of the International Conference on Neutron Scattering, to be held in Knoxville, USA, between 3-7 May.

The nominations received for the 2009 Walter Hälg Prize were examined by an international selection committee consisting of authorities representing the major scientific disciplines, both within and beyond the field of neutron scattering. After considerable deliberations the selection committee is now delighted to announce that the recipient of the 2009 Walter Hälg Prize will be

Professor Dieter Richter

of the Research Center Jülich, Germany, in recognition of his coherent work towards understanding the dynamics of polymers and biological macromolecules using high-resolution neutron scattering techniques.

Dieter Richter’s work is best known for his seminal contributions to the understanding of the dynamics of polymers on various length and time scales. In his early work the scaling predictions of the Zimm model were verified unambiguously, and relevant deviations from the Rouse model were found indicating the importance of topological constraints (Walter Schottky Award 1987). Later he succeeded to prove the molecular existence of reptation of polymer chains, which was predicted theoretically by the Nobel laureate de Gennes. Further work dealt with the understanding of the glass transition by identifying the relevant dynamic processes such as local motions, vibrations, and relaxation effects. Conveying his polymer dynamics approach to proteins, recently he successfully observed functionally important collective protein motions in space and time. His work also had an impact on industrial applications; in particular, the study of polymer aggregates with crystalline cores has lead to the development and microscopic explanation of the function of new diesel additives, which prevent the formation of large wax crystals in diesel vehicles in winter. Another important exploit was the discovery and molecular understanding of the efficiency boosting effect of amphiphilic polymers in microemulsions, which led to environmentally friendly industrial cleaners (Schrödinger Award 2002). In the course of his scientific work he continuously pushed high-resolution neutron spectroscopy to its limits, culminating in a spin-echo spectrometer reaching the micro-second time scale, which will open new horizons in the study of large macromolecules relevant for biology.

Dieter Richter graduated from the Technical University of Aachen, Germany, in 1977. Afterwards he spent one year as postdoctoral scientist in the group of Gen Shirane at the Brookhaven National Laboratory (USA). From 1979-1984 he held a scientist position at the Research Center Jülich, and from 1985-1989 he was senior scientist at the Institute Laue-Langevin Grenoble where he developed high-resolution neutron spectroscopic techniques. In 1989 he was appointed as a director at the Institute for Solid State Research of the Research Center Jülich, combined with a chair in physical chemistry at the University of Münster. He was one of the founders of the European Neutron Scattering Association and its first chairman from 1994-1997.

Announcements

SGN/SSDN Members

The Swiss Neutron Scattering Society welcomes the following new members:

- Malte Hildebrandt,
  Paul Scherrer Institut, Switzerland
- Berno Spiegelhalder,
  Astrium GmbH, Germany
- Herma Büttner,
  ANSTO, Australia

Presently the SGN has 200 members. Online registration for new members of our society is available from the SGN website: http://sgn.web.psi.ch

SGN/SSDN Annual Member Fee

The SGN/SSDN members are kindly asked to pay their annual member fees. The fee is still **CHF 10.–** and can be paid either by bank transfer or in cash during your next visit at PSI. The bank account of the society is accessible for both Swiss national and international bank transfers. The coordinates are as follows: Postfinance: 50-70723-6 (BIC: POFICHBE), IBAN: CH39 0900 0000 5007 0723 6

Joint Users' Meeting at PSI: JUM@P '09

Please remember the first joint users' meeting (JUM@P '09) of the PSI user facilities on **October 12-13, 2009.** The registration is still open until September 15, 2009. More information can be obtained here: http://user.web.psi.ch/jump09

PSI Facility News

PSI launched a **quarterly electronic newsletter** featuring recent news, events and scientific highlights of the three major PSI user facilities SLS, SINQ and SμS. The online version of the recent edition (II/09) is available here: http://user.web.psi.ch/newsletter/09-02/

SINQ Call for Proposals

The next **deadline** for the submission of beam time requests for the Swiss spallation neutron source 'SINQ' (http://sinq.web.psi.ch) will be: **November 15, 2009**

Registration of publications

Please remember to **register all publications either based on data taken at SINQ, SLS, SμS or having a PSI co-author** to the Digital User Office: https://duo.psi.ch. Please follow the link 'Publications' from your DUO main menu.

Open Positions at ILL

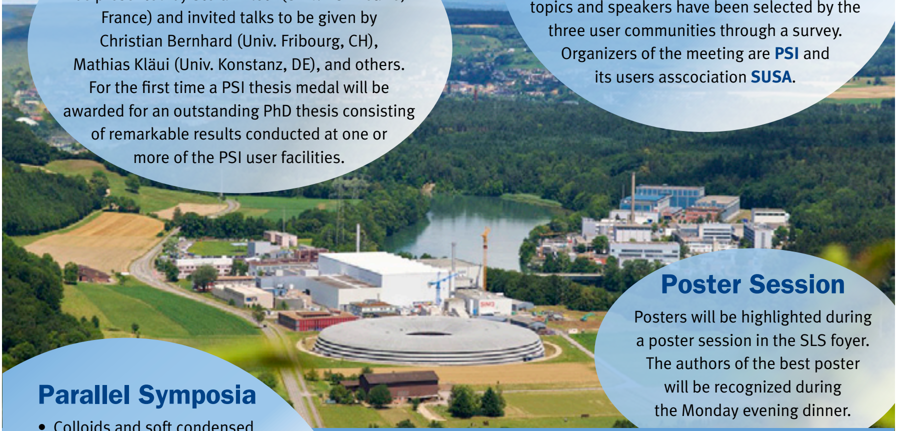
To check the open positions at ILL please have a look at the following ILL-Webpage: http://www.ill.eu/careers

PAUL SCHERRER INSTITUT

JUM@P '09
Joint Users' Meeting at PSI 2009

October 12–13, 2009

Paul Scherrer Institut, Villigen, Switzerland



Scope

The Paul Scherrer Institut operates on one campus three major user facilities for condensed matter research: The Swiss Light Source **SLS**, the Swiss Spallation Neutron Source **SINQ** and the Swiss Muon Source **SμS**. JUM@P '09 is a *"by users, for users"* meeting. Both topics and speakers have been selected by the three user communities through a survey. Organizers of the meeting are **PSI** and its users asscociation **SUSA**.

Plenary Session

The program includes a keynote lecture to be presented by Stefan Klotz (Univ. P&M Curie, France) and invited talks to be given by Christian Bernhard (Univ. Fribourg, CH), Mathias Kläui (Univ. Konstanz, DE), and others. For the first time a PSI thesis medal will be awarded for an outstanding PhD thesis consisting of remarkable results conducted at one or more of the PSI user facilities.

Poster Session

Posters will be highlighted during a poster session in the SLS foyer. The authors of the best poster will be recognized during the Monday evening dinner.

Parallel Symposia

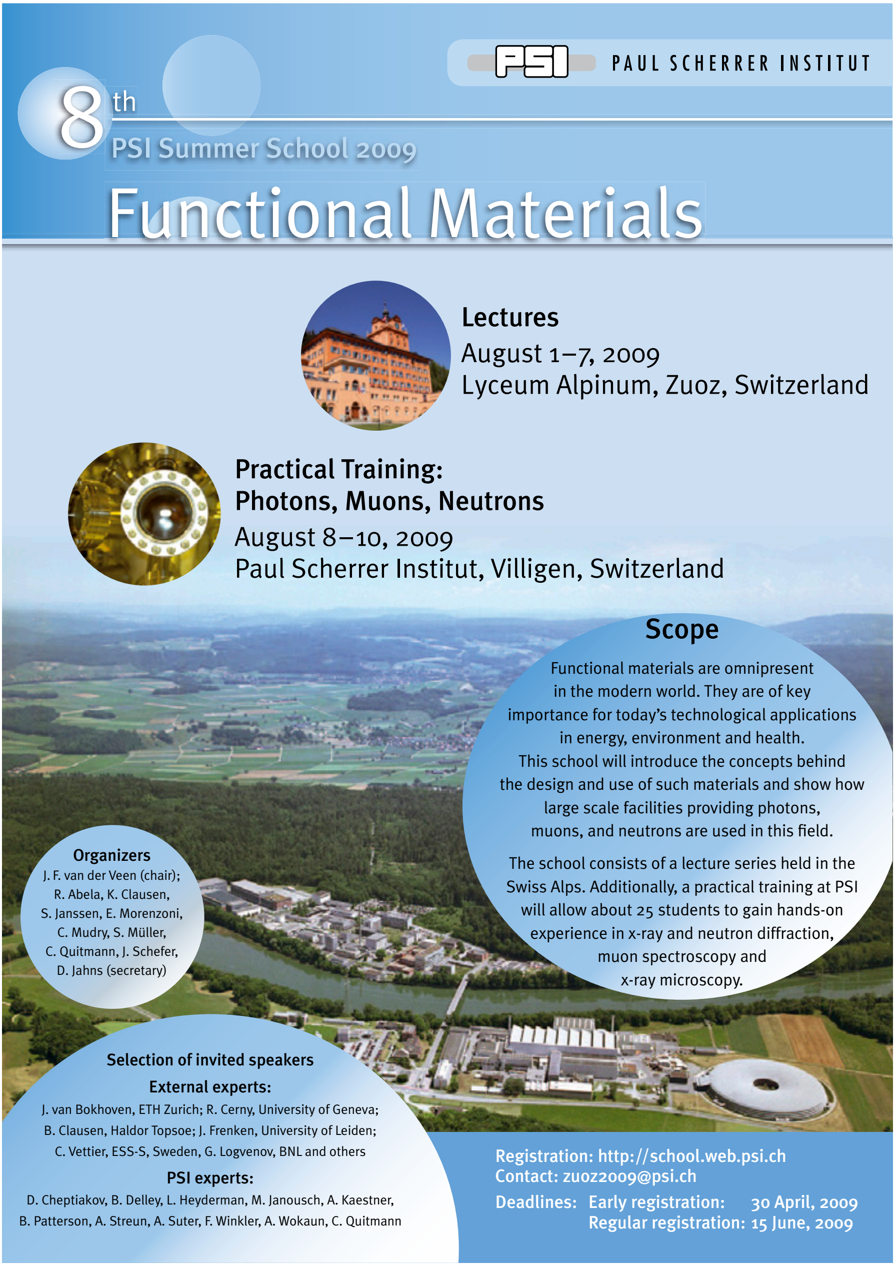
- Colloids and soft condensed matter
- Correlated electron systems
- Materials for environment and energy
- Imaging of biological and technical materials
- Advanced techniques at PSI large facilities
- From gene to structure: impact of automation technologies

Organizers: Paul Scherrer Institut, PSI Users' Association

Registration: http://user.web.psi.ch/jump09
Contact: slsuo@psi.ch

Deadlines:

Submission of abstracts for oral presentations	**extended to July 15**
Application for grants (Master and PhD students only, poster presentation mandatory)	August 31
Submission of abstracts for poster presentations	September 15
Registration	September 15



PAUL SCHERRER INSTITUT

8th

PSI Summer School 2009

Functional Materials

Lectures

August 1–7, 2009
Lyceum Alpinum, Zuoz, Switzerland

Practical Training: Photons, Muons, Neutrons

August 8–10, 2009
Paul Scherrer Institut, Villigen, Switzerland

Scope

Functional materials are omnipresent in the modern world. They are of key importance for today's technological applications in energy, environment and health. This school will introduce the concepts behind the design and use of such materials and show how large scale facilities providing photons, muons, and neutrons are used in this field.

The school consists of a lecture series held in the Swiss Alps. Additionally, a practical training at PSI will allow about 25 students to gain hands-on experience in x-ray and neutron diffraction, muon spectroscopy and x-ray microscopy.

Organizers

J. F. van der Veen (chair); R. Abela, K. Clausen, S. Janssen, E. Morenzoni, C. Mudry, S. Müller, C. Quitmann, J. Schefer, D. Jahns (secretary)

Selection of invited speakers

External experts:

J. van Bokhoven, ETH Zurich; R. Cerny, University of Geneva; B. Clausen, Haldor Topsoe; J. Frenken, University of Leiden; C. Vettier, ESS-S, Sweden, G. Logvenov, BNL and others

PSI experts:

D. Cheptiakov, B. Delley, L. Heyderman, M. Janousch, A. Kaestner, B. Patterson, A. Streun, A. Suter, F. Winkler, A. Wokaun, C. Quitmann

Registration: http://school.web.psi.ch
Contact: zuoz2009@psi.ch

Deadlines: Early registration: 30 April, 2009
Regular registration: 15 June, 2009

Conferences and Workshops 2009/10

JULY

ICM 2009: 18th International Conference on Magnetism
July 26–31, 2009, Karlsruhe, Germany

International Conference on ‚Energy materials research using neutron and synchrotron radiation'
July 27–30, 2009, Berlin, Germany

AUGUST

8th PSI Summer School on Condensed Matter Research 2009: Functional Materials
August 1–10, 2009, Zuoz, Switzerland

Polarized Neutrons and Synchrotron X-rays for Magnetism 2009
August 2–5, 2009, Bonn, Germany

Sagamore XVI: Charge, Spin and Momentum Densities, includes sessions on Neutron Scattering, Ultrafast Time-Resolved Studies and the Electronic Structure of Nanoparticles
August 2–7, 2009, Santa Fe, USA

2nd AONSA Neutron School 2009
August 16–21, 2009, Lucas Heights (Sydney), Australia

ECM 25: 25th European Crystallographic Meeting
August 16–21, 2009, Istanbul, Turkey

Perovskites – Properties and Potential Applications
August 16–21, 2009, Cancun, Mexico

MRC XVIII: International Materials Research Congress
August 16–21, 2009, Cancun, Mexico

Diffusion Fundamentals III
August 23–26, 2009, Athens, Greece

ICHMS 2009: XI International Conference on Hydrogen Materials Science and Chemistry of Carbon Nanomaterials
August 25–31, 2009, Yalta-Crimea, Ukraine

Scoping workshop 2009 For New Guides, Instruments and Sample-Environment Apparatus at OPAL
August 27–28, 2009, ANSTO, Sydney, Australia

11th Oxford School on Neutron Scattering
August 31 – September 12, 2009, Oxford, United Kingdom

SEPTEMBER

Annual Meeting of the Swiss Physical Society
September 2–4, 2009, Innsbruck, Austria

9th International Conference on Materials and Mechanics of Superconductivity
September 7–12, 2009, Tokyo, Japan
X School on Synchrotron Radiation: Fundamentals, Methods and Applications
September 7–18, 2009, Trieste, Italy

SRPS 4: Synchrotron Radiation in Polymer Science
September 8–11, 2009, Kerkrade, The Netherlands

SAS-2009: XIV International Conference on Small-Angle Scattering
September 13–18, 2009, Rutherford Appleton Laboratory, Oxford, United Kingdom

GISAS satellite conference
September 20–23, 2009, DESY, Hamburg, Germany

OffSpec: Theory and Data Analysis for Grazing Incidence and Off-Specular Scattering
September 27–29, 2009, Feldafing, Germany

OCTOBER

SKIN2009: Studying Kinetics with neutrons (SANS and Reflectometry) October 5–7, 2009, Grenoble, France

JCNS Workshop 2009: Trends and Perspectives in Neutron Scattering on Soft Matter October 5–8, 2009, Tutzing, Germany

HZB Orbital Workshop 2009
October 7–8, 2009, Berlin, Germany

JUM@P 09: Joint Users' Meeting at PSI
October 12–13, 2009, Paul Scherrer Institut, Villigen, Switzerland

AIC Information Day on Large Facilities
October 19, 2009, Paul Scherrer Institut, Villigen, Switzerland

2010:

JANUARY

5th SOLEIL Users Meeting
January 20–21, 2010, Synchrotron Soleil, Gif-sur-Yvette, France

Flipper 2010: International Workshop on Single-Crystal Diffraction with Polarised Neutrons
January 27–29, 2010, Grenoble, France

MARCH

ICANS-XIX: The 19th Meeting of the International Collaboration on Advanced Neutron Sources
March 8–12, 2010, Grindelwald, Switzerland

HERCULES XX: HERCULES Symposium
March 25–26, 2010, Grenoble, France

APRIL

MRS Symposium W: Diagnostics and Characterization of Energy Materials with Synchrotron and Neutron Radiation
April 5–9, 2010, San Francisco, USA

JUNE

RCBJSF-10: The 10th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity
June 20–25, 2010, Yokohama, Japan

JULY

PNCMI 2010: 8th International Workshop on Polarised Neutrons in Condensed Matter Investigations
July 5–8, 2010, Delft, The Netherlands

OCTOBER

WCNR-9: 9th World Congress on Neutron Radiography
October 3–8, 2010, Kwa-Maritane, South Africa

(an updated list with online links can be found here: http://sinq.web.psi.ch/sinq/links.html)

Swiss Neutron Scattering Society
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